

Theoretical Study on Transport Properties of Normal Metal - Zigzag Graphene Nanoribbon - Normal Metal Junctions

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We investigate transport properties of the junctions in which the graphene nanoribbon with the zigzag shaped edges consisting of the N legs is sandwiched by the two normal metals by means of recursive Green's function method. The conductance and the transmission probabilities are found to have the remarkable properties depending on the parity of N . The singular behaviors close to $E = 0$ with E being the Fermi energy are demonstrated. The channel filtering is shown to occur in the case with $N = \text{even}$.

KEYWORDS: graphene nanoribbon, zigzag shaped edges, transport property

Recently, graphene-based materials with nano-meter sizes have been attracting much attention in both fundamental and applied sciences. Among these materials, the graphene nanoribbon with zigzag shaped edges, which is abbreviated to zigzag GNR in the following, has fascinating peculiar properties as follows.¹⁻³ The zigzag GNR has a metallic band structure irrespective of the width N in the sense that the energy gap does not appear at the Fermi energy in the absence of doping, $E = 0$. However, the asymptotic form of the energy dispersion near $E = 0$ is written as $E \propto \pm |k - \pi/a|^N$ with a being the lattice spacing and then Drude weight in the absence of doping becomes zero due to the vanishing Fermi velocity for $N \geq 2$. Therefore, according to Kohn's criterion,⁴ the system without doping is classified into the insulator from the point of view for transport properties. Such characteristic properties are due to the fact that the one-particle states near $E = 0$ are localized around zigzag edges.

Transport properties of the zigzag GNR applied to the external potential have been studied theoretically,⁵⁻⁸ and it has been found that the parity of the width N remarkably affects the transport properties. In the case of $N = \text{even}$, the zigzag GNR has the reflection symmetry in the transverse direction, and as a result, the parity of the wave function in the direction must be even or odd. Since only the scattering processes conserving the parity of the wave function are allowed under the external potential not varying in the transverse direction, the filtering of the scattering processes happens depending on the parity of the wave function of the transverse direction.⁸ Note that such an interesting phenomenon depending on the parity of the width N have been found in the persistent current of the isolated ring pierced by the magnetic flux.⁹ However, the transport properties of the junctions which consist of the zigzag GNR and the normal metals have not been investigated.

In the present paper, we investigate the transport properties of the junctions shown Fig. 1 where the zigzag GNR with the width N and the length $2N_L$ is sandwiched by the two ideal leads expressed by the regular

square lattices. The Hamiltonian is written as follows,

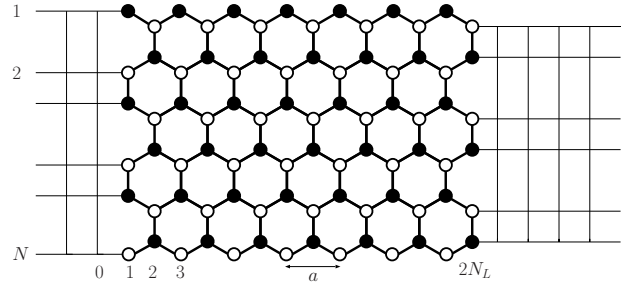


Fig. 1. The present model where the zigzag GNR written by the thick lines is sandwiched by the ideal leads expressed by the regular square lattices, which is expressed by the thin lines. Here, the width and length are given by N and $2N_L$, respectively, and a is the lattice spacing of the zigzag GNR. The filled (open) circles in the zigzag GNR region express the A (B) sublattice.

$$H = \sum_{i,j} t_{i,j} |i\rangle \langle j|, \quad (1)$$

where $|i\rangle$ is the localized state at the site i and $t_{i,j} = -t$ if i and j are nearest neighbors, otherwise $t_{i,j} = 0$. The hopping in the GNR region is assumed to have the same value t as that in the normal metals for simplicity. The conductance in unit of $2e^2/h$ ($-e < 0$: electronic charge, h : Planck constant), g , written by Landauer formula

$$g = \sum_{\mu,\nu} T_{\mu,\nu} \quad (2)$$

is calculated by the recursive Green's function method.¹⁰ Here, $T_{\mu,\nu}$ is the transmission probability from the incident channel ν to transmitted one μ , both of which are defined in the ideal leads. Note that we have confirmed that the conservation law $\sum_{\mu} \{T_{\mu,\nu} + R_{\mu,\nu}\} = 1$ holds in all the numerical calculation in order to check validity of our results where $R_{\mu,\nu}$ is the reflection probability from the channel ν to μ .

At first, the cases without doping, i.e., $E/t = 0$ are discussed.¹¹ We show the conductance g as a function of the length N_L for $N = \text{even}$ in Fig. 2 (a) and $N = \text{odd}$ in

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Fig. 2 (b), respectively. We can observe obvious qualita-

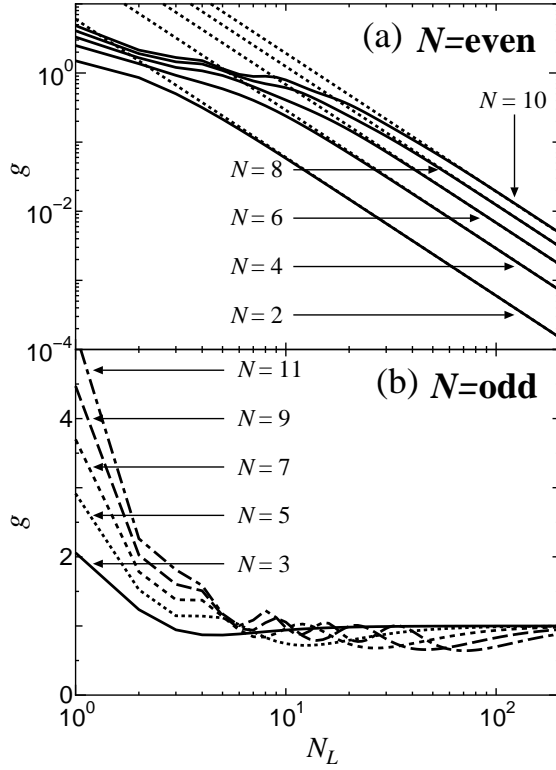


Fig. 2. The conductance g at $E/t = 0$ as a function of N_L for $N = 2, 4, 6, 8, 10$ (a) and for $N = 3, 5, 7, 9, 11$ (b). In (a), the dotted lines express the asymptotic behaviors for $N_L \gg 1$, all of which are proportional to N_L^{-2} .

tive discrepancy between $N = \text{odd}$ and $N = \text{even}$ in the asymptotic behavior for $N_L \gg 1$. In the case with $N = \text{odd}$, the conductances approach to unity, which indicates that only the one channel survives in the limit. On the other hand, those for $N = \text{even}$ decrease in proportion to N_L^{-2} . Actually, we can successfully derive the expression $g \simeq 6/N_L^2$ by obtaining the recursive Green's function analytically in the case of $N = 2$. Note that the transmission probabilities are obtained as $T_{1,1} = T_{2,2} \simeq 3/N_L^2$ and $T_{1,2} = T_{2,1} \simeq 0$ in this limit.

Next, the cases with $E/t \neq 0$ are investigated. Due to the particle-hole symmetry, the transport properties for $E/t > 0$ are the same as those for $E/t < 0$. Therefore we concentrate on only the $E/t > 0$ cases unless explicitly noted. In addition, we discuss the energy regions where the one band gets across the Fermi energy. Here, there exists the one-to-one correspondence between the energy and the Fermi wavenumber k_F ; k_F is equal to π/a at $E/t = 0$ and decreases with increasing the energy. Therefore, the conductances are investigated as a function of the Fermi wavenumber instead of the energy. In Fig. 3, we show the conductances as a function of $2k_FL/\pi$ for $N = \text{even}$ (a) and $N = \text{odd}$ (b) with the fixed length $N_L = 200$. In this analysis, we use $L = (N_L + 1/2)a$ as the length of the zigzag GNR region L . In each figure, the right end of the horizontal axis is given by $2k_FL/\pi = 401$ and it corresponds to $E/t = 0$, i.e., $k_F = \pi/a$. We can

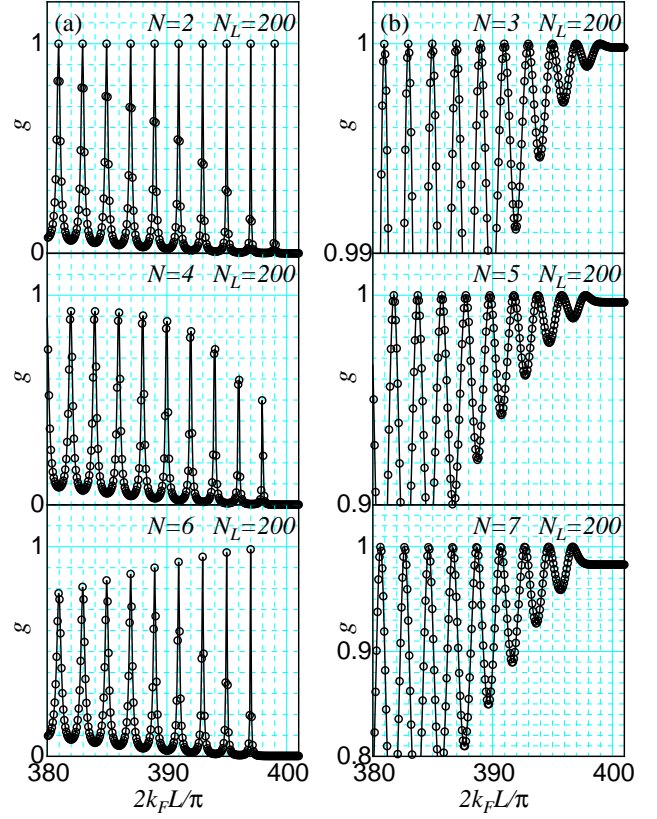


Fig. 3. (Color online) The conductance g at $E/t > 0$ as a function of $2k_FL/\pi$ for $N = \text{even}$ (a) and for $N = \text{odd}$ (b) with $L = (N_L + 1/2)a$ being the length of the zigzag GNR region and $N_L = 200$. In each figure, the right end of horizontal axis $2k_FL/\pi = 401$ corresponds to the $E/t = 0$ case.

see the oscillating behavior in the both cases except near $E/t = 0$. The interval between one peak and the nearest neighbor one is given by $\Delta(k_FL) = \pi$. Therefore, the oscillation is considered to be originated from the interference between the electron waves at the Fermi energy. It should be noted that such oscillating behavior disappears near $E/t = 0$. In the cases of $N=2$ and 3 (4 and 5), the peak which should appear at $2k_FL/\pi = 401(400)$ does not exist. With increasing the width of the zigzag GNR, the number of missing peaks increase. For example, the two peaks expected at $2k_FL/\pi = 399$ and 401 respectively are missing in the cases of $N = 6$ and 7.

Here, the transmission probabilities $T_{\mu,\nu}$ are discussed in detail for the $N = \text{even}$ cases. In these cases, as was already noted, the band selective filtering is known to occur in the transport properties of zigzag GNR under the external potential uniform in the transverse direction.⁸ The origin of the filtering is the reflection symmetry in the transverse direction, which makes the wave function in the direction either even or odd function. Since the present external leads has also reflection symmetry, the wave function of the channel defined in the external leads is either the even or odd function. Therefore, the filtering depending on the channel indices is expected for the $N = \text{even}$ cases. We show the transmission probability $T_{\mu,\nu}$ for $N = 4$ as a function of N_L for $E/t = 0.1$ (a), $E/t = -0.1$ (b) and $E/t = 0.0$ (c) in Fig. 4. In the case

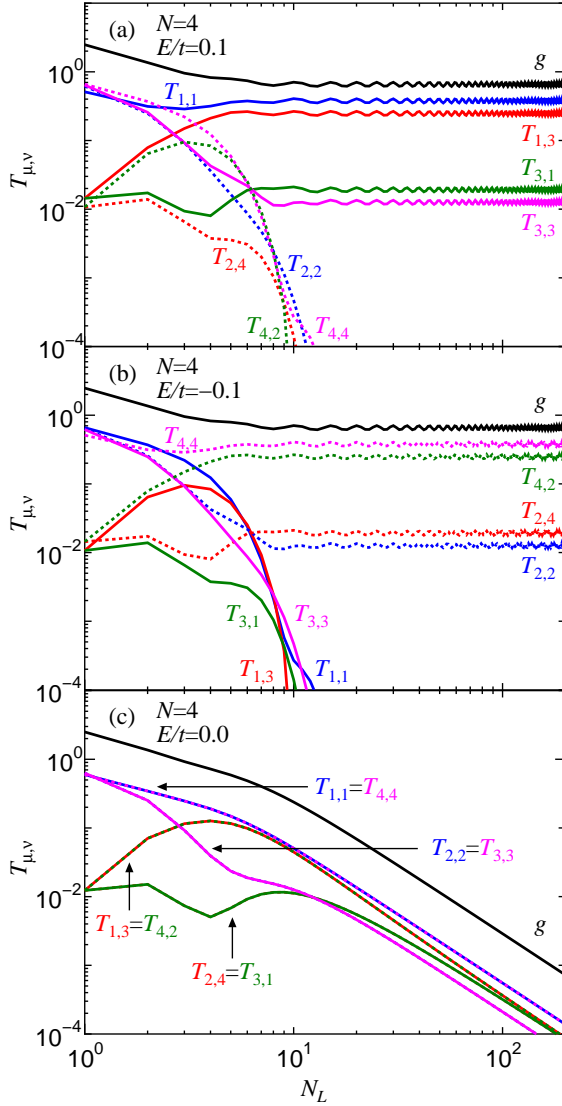


Fig. 4. (Color online) The transmission probability $T_{\mu,\nu}$ together with the conductance g for $N = 4$ as a function of N_L in the cases of $E/t = 0.1$ (a), $E/t = -0.1$ (b) and $E/t = 0.0$ (c).

of $E/t = 0.1$, the transmission probabilities $T_{\text{odd,odd}}$ becomes finite for $N_L \gg 1$, whereas only $T_{\text{even,even}}$ survives for $E/t = -0.1$. The other transmission processes such as those from the even channel to the odd one and vice versa are suppressed in the both cases. These results can be understood in terms of the parity of the wave function in the transverse direction; The wave function of the channel μ , $u_\mu(l)$ ($l = 1, 2, \dots, N$), in the external leads is given as follows,

$$u_\mu(l) = \sqrt{\frac{2}{N+1}} \sin k_y(\mu)l, \quad (3)$$

$$k_y(\mu) = \frac{\mu\pi}{N+1}, \quad (\mu = 1, 2, \dots, N) \quad (4)$$

and its parity is positive for $\mu = \text{odd}$, whereas negative for $\mu = \text{even}$. On the other hand, in the zigzag GNR with the width $N = \text{even}$, among the two bands located around $E/t = 0$ the wave function for $E/t > 0$ is the even function in the transverse direction, whereas that

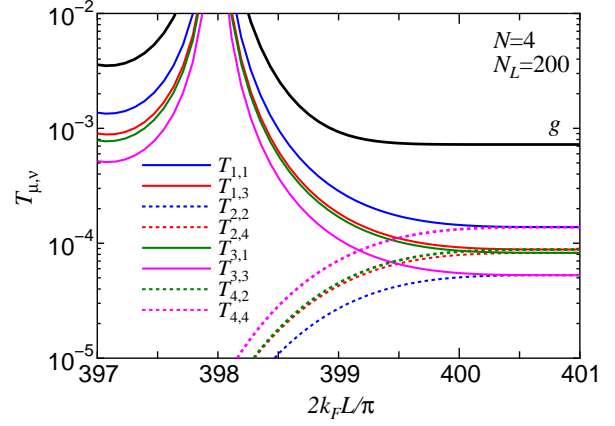


Fig. 5. (Color online) The transmission probability $T_{\mu,\nu}$ together with the conductance g for $N = 4$ and $N_L = 200$ as a function of $2k_F L/\pi$. The right end of the horizontal axis $2k_F L/\pi = 401$ corresponds to $E/t = 0$.

for $E/t < 0$ is the odd one.⁸ Since the parity of the wave function in the transverse direction should be conserved when passing through the zigzag GNR, the channels with positive (negative) parity can pass through for $E/t > 0$ ($E/t < 0$). At $E/t = 0.0$, the two bands touch with each other and two states are degenerate. Therefore, the two kinds of channels, *i.e.*, from even to even and from odd to odd, are alive in the case of $E/t = 0.0$. Actually, the analytical calculation for $N = 2$, $T_{1,1} = T_{2,2} \simeq 3/N_L^2$ supports the conclusion shown above.

Now, we investigate this channel filtering in detail close to $E/t = 0$ where, as has been already discussed above, the anomalous phenomenon that the oscillation of g as a function of $k_F L$ disappears is observed. In Fig. 5, the transmission probabilities for $N = 4$ and $N_L = 200$ are shown as a function of $2k_F L/\pi$ as well as the conductance g . Here, the $E/t \gtrsim 0$ case is discussed and the right end of the horizontal axis corresponds to $E/t = 0.0$. The last peak in the conductance oscillation is observed at $2k_F L/\pi = 398$ and the peak which should be observed at $2k_F L/\pi = 400$ diminishes. In the region, we can see that the transmission processes from the even channel to the even one, which is prohibited due to parity conservation, become possible. The regions where the oscillation disappears correspond to those with the breakdown of the parity conservation. Therefore, the two phenomena can be considered to come from the same origin.

Though discussed that the energy levels of the finite system attached to the leads are shifted by the amount of \hbar/τ , where τ is the time it takes for an electron to move to the end of the system.¹² The conductance can be understood from the point of view that the states within the shift can pass through the sample.¹³ Though he discussed the case with random impurities where the motion of the electron is diffusive, such a shift of the energy levels in the GNR region of the present system can be expected to occur in the presence of the ideal leads. As a result, the anomalous phenomena seen in $E/t = 0$ can be expanded to the $E/t \neq 0$ region. However, at present, it is unclear why the conductance at $E/t \simeq 0$

shows the discrepancy in the N_L dependences between $N = \text{even}$ and $N = \text{odd}$ case. It is likely that the discrepancy in the transport properties originates from that in coupling between the GNR and the normal metal because the qualitative difference between $N = \text{even}$ and $N = \text{odd}$ cannot be observed in the band structure of the isolated GNR. Further investigation on the electronic states of GNR attached with the ideal leads is necessary in order to understand the transport properties of the normal metal - zigzag GNR - normal metal junctions.

In conclusion, we investigated the transport properties of the junction where the zigzag GNR with width N and length $2N_L$ is sandwiched by the normal metals expressed by the regular square lattices. The transport property at $E/t = 0$ shows different asymptotic behavior as the a function of N_L , *i.e.*, for $N_L \gg 1$ the conductance with $N = \text{odd}$ approaches to unity whereas that in the case of $N = \text{even}$ decreases in proportion to N_L^{-2} . The conductance at $E/t \neq 0$ shows oscillating behavior as a function of the energy, which is due to the interference of the electron wave at the Fermi energy. Such a oscillation disappears close to $E/t = 0$. In addition, the channel filtering occur in the case of $N = \text{even}$ with the reflection symmetry in the transverse direction. The filtering is found also to show unexpected behavior close

to $E/t = 0$.

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